

ABSTRACT OF THE DISCLOSURE

A computer implemented method modifies an experimental electron
5 density map. A set of selected known experimental and model electron density
maps is provided and standard templates of electron density are created from the
selected experimental and model electron density maps by clustering and
averaging values of electron density in a spherical region about each point in a
grid that defines each selected known experimental and model electron density
10 maps. Histograms are also created from the selected experimental and model
electron density maps that relate the value of electron density at the center of each
of the spherical regions to a correlation coefficient of a density surrounding each
corresponding grid point in each one of the standard templates. The standard
templates and the histograms are applied to grid points on the experimental
15 electron density map to form new estimates of electron density at each grid point
in the experimental electron density map.